

Please amend claims 1, 3-4 and add new claims 5-20. Pursuant to 37 C.F.R. 1.121(b), Applicant is attaching a clean form of the pages showing the amended claims as now pending, and another version marked to show all the changes relative to the previous version of the claims pages.

#### REMARKS

This is a resubmission of the applicant's previous response to the Office Action dated March 16, 2001, reformatted pursuant to the Office Action dated June 25, 2001.

The applicant responds to the Office Action dated March 16, 2001, and overcomes each of the examiner's grounds for rejection of and objection to the claims, objections to the specification, and objections to the drawings. The applicant will set forth in specificity each of his bases for overcoming the examiner's rejections and objections.

Claims 1-4 have been amended and new dependent claims 5-20 have been added. The claims are directed to a method, a system, and software for use in deriving chemical structural information. A chemical name is acquired that lacks an association with a chemically accurate computer readable diagrammatic representation of a substance identified by the chemical name. The chemical name is parsed into at least first and second fragments that are non-contiguous. Computer executable logic is applied to the first and second fragments. The computer executable logic determines, based at least in part on the positions of the first and second fragments within the chemical name, respective first and second chemically accurate computer readable diagrammatic representations of the first and second fragments.

Claim 1, 3-4 have been amended to make more clear that the chemical name recited in the claims is a chemical name lacking an association with a chemically accurate computer readable diagrammatic representation of a substance identified by the chemical name, and that the diagrammatic representations that are determined are of non-contiguous fragments based at least in part on the positions of the non-contiguous fragments.

The examiner has objected to the title. The title has been amended to address the examiner's objection.



**Replacement Title for Page 1, line 1 of the Specification**

**(CLEAN FORM)**

--METHOD, SYSTEM, AND SOFTWARE FOR DERIVING  
CHEMICAL STRUCTURAL INFORMATION--



**Replacement Title for Page 1, line 1 of the Specification**

**(MARKED TO SHOW CHANGES)**

**--METHOD, SYSTEM, AND SOFTWARE FOR DERIVING  
CHEMICAL STRUCTURAL INFORMATION--**



Replacement Pages for Claims 1, 3-20

(CLEAN FORM)

SUB 1  
B1

1. A method for use in deriving chemical structural information, comprising:

acquiring a chemical name lacking an association with a chemically accurate computer readable diagrammatic representation of a substance identified by the chemical name;

parsing the chemical name into at least first and second fragments, the first and second fragments being non-contiguous; and

applying computer executable logic to the first and second fragments, the computer executable logic determining, based at least in part on the positions of the first and second fragments within the chemical name, respective first and second chemically accurate computer readable diagrammatic representations of the first and second fragments.

SUB 2  
B2

3. A system for use in deriving chemical structural information, comprising:

an acquiror acquiring a chemical name lacking an association with a chemically accurate computer readable diagrammatic representation of a substance identified by the chemical name;

a parser parsing the chemical name into at least first and second fragments, the first and second fragments being non-contiguous; and

computer executable logic determining, based at least in part on the positions of the first and second fragments within the chemical name, respective first and second chemically accurate computer readable diagrammatic representations of the first and second fragments.

4. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive chemical structural information, the instructions causing the system to:

acquire a chemical name lacking an association with a chemically accurate computer readable diagrammatic representation of a substance identified by the chemical name;

parse the chemical name into at least first and second fragments, the first and second fragments being non-contiguous; and

apply computer executable logic to the first and second fragments, the computer executable logic determining, based at least in part on the positions of the first and second fragments within the chemical name, respective first and second chemically accurate computer readable diagrammatic representations of the first and second fragments.

5. The method of claim 1, further comprising:

making a change to the chemical name to facilitate subsequent analysis of the chemical name.

6. The method of claim 1, further comprising:

detecting that the chemical name has an inverted form; and  
changing the chemical name to an uninverted form.

7. The method of claim 1, further comprising:

inserting a delimiter into the chemical name.

8. The method of claim 1, further comprising:

comparing at least one of the first and second fragments to at least a portion of the contents of a set of chemical characteristics data.

9. The method of claim 8, further comprising:

associating at least one of the first and second fragments with a data object belonging to the set of chemical characteristics data.

10. The method of claim 9, wherein the data object includes a connection table.

11. The method of claim 9, wherein the data object includes a locant map.

12. The method of claim 9, wherein the data object includes an attach-in map.

13. The method of claim 9, wherein the data object includes an attach-out map.

14. The method of claim 8, further comprising:

selecting the portion of the contents as being representative of at least one of the first and second fragments; and

rejecting the portion of the contents in favor of another portion of the contents.

15. The method of claim 9, further comprising:

deriving at least one of the first and second chemically accurate computer readable diagrammatic representations from information belonging to the data object.

16. The computer software of claim 4, further comprising instructions for use in a computer system to help cause the computer system to:

make a change to the chemical name to facilitate subsequent analysis of the chemical name.

17. The computer software of claim 4, further comprising instructions for use in a computer system to help cause the computer system to:

detect that the chemical name has an inverted form; and

change the chemical name to an uninverted form.

18. The computer software of claim 4, further comprising instructions for use in a computer system to help cause the computer system to:

insert a delimiter into the chemical name.

19. The computer software of claim 4, further comprising instructions for use in a computer system to help cause the computer system to:

compare at least one of the first and second fragments to at least a portion of the contents of a set of chemical characteristics data.

B3 20. The computer software of claim 19, further comprising instructions for use in a computer system to help cause the computer system to:

associate at least one of the first and second fragments with a data object belonging to the set of chemical characteristics data.

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**Replacement Claims for Claims 1, 3-20**

**(MARKED TO SHOW CHANGES)**

- 1. A method for use in deriving chemical structural information, comprising:
- acquiring a chemical name lacking an association with a chemically accurate computer readable diagrammatic representation of a substance identified by the chemical name;
- parsing [a] the chemical name into at least first and second fragments, the first and second fragments being non-contiguous; and
- applying computer executable logic to the first and second fragments, the computer executable logic determining, based at least in part on the positions of the first and second fragments within the chemical name, respective first and second chemically accurate computer readable diagrammatic representations of the first and second fragments.
3. A system for use in deriving chemical structural information, comprising:
- an acquiror acquiring a chemical name lacking an association with a chemically accurate computer readable diagrammatic representation of a substance identified by the chemical name;
- a parser parsing [a] the chemical name into at least first and second fragments, the first and second fragments being non-contiguous; and
- [a determiner] computer executable logic determining, based at least in part on the positions of the first and second fragments within the chemical name, respective first and second chemically accurate computer readable diagrammatic representations of the first and second fragments.



4. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive chemical structural information, the instructions causing the system to:

acquire a chemical name lacking an association with a chemically accurate computer readable diagrammatic representation of a substance identified by the chemical name;

parse [a] the chemical name into at least first and second fragments, the first and second fragments being non-contiguous; and

apply computer executable logic to the first and second fragments, the computer executable logic determining [determine], based at least in part on the positions of the first and second fragments within the chemical name, respective first and second chemically accurate computer readable diagrammatic representations of the first and second fragments.

5. The method of claim 1, further comprising:

making a change to the chemical name to facilitate subsequent analysis of the chemical name.

6. The method of claim 1, further comprising:

detecting that the chemical name has an inverted form; and  
changing the chemical name to an uninverted form.

7. The method of claim 1, further comprising:

inserting a delimiter into the chemical name.

8. The method of claim 1, further comprising:

comparing at least one of the first and second fragments to at least a portion of the contents of a set of chemical characteristics data.

9. The method of claim 8, further comprising:

associating at least one of the first and second fragments with a data object belonging to the set of chemical characteristics data.

10. The method of claim 9, wherein the data object includes a connection table.

11. The method of claim 9, wherein the data object includes a locant map.

12. The method of claim 9, wherein the data object includes an attach-in map.

13. The method of claim 9, wherein the data object includes an attach-out map.

14. The method of claim 8, further comprising:

selecting the portion of the contents as being representative of at least one of the first and second fragments; and

rejecting the portion of the contents in favor of another portion of the contents.

15. The method of claim 9, further comprising:

deriving at least one of the first and second chemically accurate computer readable diagrammatic representations from information belonging to the data object.

16. The computer software of claim 4, further comprising instructions for use in a computer system to help cause the computer system to:

make a change to the chemical name to facilitate subsequent analysis of the chemical name.

17. The computer software of claim 4, further comprising instructions for use in a computer system to help cause the computer system to:

detect that the chemical name has an inverted form; and

change the chemical name to an uninverted form.

18. The computer software of claim 4, further comprising instructions for use in a computer system to help cause the computer system to:

insert a delimiter into the chemical name.

19. The computer software of claim 4, further comprising instructions for use in a computer system to help cause the computer system to:

compare at least one of the first and second fragments to at least a portion of the contents of a set of chemical characteristics data.

20. The computer software of claim 19, further comprising instructions for use in a computer system to help cause the computer system to:

associate at least one of the first and second fragments with a data object belonging to the set of chemical characteristics data.--

Claims 1-4 have been rejected under 35 U.S.C. 112, first paragraph. The examiner has stated: "the specification, while being enabling for methods beginning with the uninverting of the chemical name, does not reasonably provide enablement for methods that lack said inversion."

The applicant respectfully submits that the specification enables a person skilled in the art to make the invention commensurate in scope with the claims. The specification describes an example embodiment of an invention recited in the claims, and clearly states, at page 29, line 17, that "[o]ther embodiments are within the scope of the ... claims." In particular, with respect to inversion, the specification describes preprocessing that is subsequently helpful in the example embodiment. However, it is plain to a person skilled in the art that preprocessing helps to reduce the number of fragments that need to be referenced subsequently, which reduction may or may not be pertinent or important in another embodiment. Indeed, the specification refers, at page 30, line 2, to an example embodiment in which "extended lists of known chemical name fragments" are used. Accordingly, the specification amply supports the scope with the claims.

Claim 2 has been rejected under 35 U.S.C. 112, first paragraph, as containing subject matter which was not described in the specification in such a way as to enable one skilled in the art to which it pertains, or with which it is most nearly connected, to make or use the invention. The examiner has stated: "[a] full consideration of the specification failed to reveal the 'conditions' that are associated with the later second 'text strings'".

The applicant respectfully submits that the specification enables a person skilled in the art to make and use the invention of claim 2. The specification describes an example embodiment of an invention recited in claim 2, in which "[e]ach known text string is associated in the lexicon with at least one data object known as a nomToken" (page 14, lines 1-2). The specification goes on to describe an example embodiment of the nomToken data object in detail, including an associated connection table and locant, attach-in, and attach-out maps (page 15, lines 1-2), which are also described in detail. It is plain to a person skilled in the art that some or all of these items may provide "conditions" as recited in claim 2. Thus, the specification provides a sufficient basis for one skilled in the art to make or use the invention.

Claims 1-4 have been rejected under 35 U.S.C. 112, second paragraph, as being indefinite for failing to particularly point out and distinctly claim the subject matter which applicant regards as the invention. The examiner has stated: "the claim, nor any other part of the application, provides the examiner with a dictionary with which to resolve the vagueness as it refers to the nomTokens."

The applicant respectfully submits that claims 1-4 are not indefinite. As stated above in connection with the discussion of the rejection of claim 2, the specification clearly describes an example embodiment of a "nomToken" and example embodiments of an associated connection table and locant, attach-in, and attach-out maps. See pages 14-17 in particular. In addition, the specification goes on to describe in detail an example of a procedure for using a nomToken data object (pages 17-30), and includes an "Appendix: NomTokens" containing examples of nomTokens. NomTokens are sufficiently explained to support claims 1-4.

Claims 1-4 have been rejected under 35 U.S.C. 102(b) as being anticipated by Ihlenfeldt et al. However, Ihlenfeldt does not disclose deriving chemical structural information where a chemical name lacks an association with a chemically accurate computer readable diagrammatic representation of a substance identified by the chemical name, as required by all of the claims as amended. A careful reading of Ihlenfeldt reveals that Ihlenfeldt pertains only to circumstances in which a chemical name or identifier is already associated with an existing "structure drawing" or "structure plot" (see, e.g., page 663, col. 2). Thus, for at least this reason, claims 1-4 are not anticipated by Ihlenfeldt.

Claims 1-4 have been rejected under 35 U.S.C. 102(e) as being anticipated by Ecker. However, Ecker does not disclose deriving chemical structural information where the diagrammatic representations that are determined are of non-contiguous fragments based at least in part on the positions of the non-contiguous fragments, as required by all the claims as amended. Ecker discloses interpreting a sequence of contiguous letters one by one in contiguous order where each letter represents a shorthand version of particular building block. Representations of building blocks are not determined based on positions of corresponding non-contiguous letters. Thus, for at least this reason, claims 1-4 are not anticipated by Ecker.

On page 6 of the examiner's action, the examiner states: "[t]his application contains an appendix consisting of a computer program listing of no more than ten (10) pages".

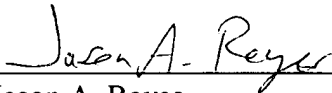
The applicant submits that the examiner is mistaken. The applicant is not aware of any appendix in the application that matches the examiner's description. The application includes two appendices: an "Appendix: NomTokens" having 111 pages, and a Microfiche Appendix having 382 frames on 4 sheets of microfiche.

The applicant submits that the application is in condition for allowance, which action is requested.

The Commissioner is hereby authorized to charge any fee deficiency, or credit any overpayment to our Deposit Account No. 08-0219.

Respectfully submitted,

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